Penalized semidefinite programming for quadratically-constrained quadratic optimization

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Abstract

In this paper, we give a new penalized semidefinite programming approach for non-convex quadratically-constrained quadratic programs (QCQPs). We incorporate penalty terms into the objective of convex relaxations in order to retrieve feasible and near-optimal solutions for non-convex QCQPs. We introduce a generalized linear independence constraint qualification (GLICQ) criterion and prove that any GLICQ regular point that is sufficiently close to the feasible set can be used to construct an appropriate penalty term and recover a feasible solution. Inspired by these results, we develop a heuristic sequential procedure that preserves feasibility and aims to improve the objective value at each iteration. Numerical experiments on large-scale system identification problems as well as benchmark instances from the library of quadratic programming demonstrate the ability of the proposed penalized semidefinite programs in finding near-optimal solutions for non-convex QCQP.

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1 Introduction

This paper studies a subclass of polynomial optimization, regarded as quadratically-constrained quadratic programming (QCQP), which is concerned with minimizing a multi-dimensional quadratic function within a feasible set that is also characterized by quadratic functions. QCQP arises in various scientific and engineering applications, such as electric power systems [52–54,56], imaging science [8,17,28,73], signal processing [2,7,19,47,50,58], automatic control [1,27,56,77], quantum mechanics [14,24,35,46], and cybersecurity [21–23,62]. The development of efficient optimization techniques and numerical algorithms for QCQP has been an active area of research for decades. Due to the barriers imposed by NP-hardness, the focus of some research efforts has shifted from designing general-purpose algorithms to specialized methods that are robust and scalable for specific application domains. Notable examples for which methods with guaranteed performance have been offered in the literature include the problems of multisensor beamforming in communication theory [31], phase retrieval in signal processing [16], and matrix completion in machine learning [15,60].

This paper advances a popular framework for the global analysis of QCQP, which involves convex hull characterization through semidefinite programming (SDP) relaxations [20,37, 44,45,59,65,66,71]. A relaxation is said to be *exact* if it has the same optimal objective value as the original problem. SDP has been critically important for constructing strong convex relaxations of non-convex optimization problems and its exactness has been verified for numerous real-world problems [13,41,43,74,75]. Additionally, in many problems for which the derivation of exact relaxations is impossible due to NP-hardness, SDP relaxations have offered effective approximation algorithms [33,34,49,64,80–83]. Geomans and Williamson [32] show that a SDP relaxation objective is within 14% of the optimal value for the MAXCUT problem on graphs with non-negative weights. Additionally, SDP relaxations are used within branch-and-bound algorithms [12,18] for finding globally optimal solutions to non-convex optimization problems.

In particular, forming hierarchies of SDP relaxations [20,37,44,45,48,59,66,71] has been proven to yield the convex hull of non-convex QCQP problems. Despite solid theoretical guarantees, one of the primary challenges for the application of SDP hierarchies beyond small-scale instances is the rapid growth of dimensionality. In response, some studies have exploited sparsity and structural patterns to boost efficiency [9,41,42,61,63]. Another direction, pursued in [1,3,6,11,55,57,68], is to use lower-complexity relaxations as alternatives to computationally demanding SDP relaxations. In this paper, we offer an alternative approach, which focuses on the penalizing the objective function of SDP relaxations as opposed to strengthening the quality of convex-hall characterization, which can be computationally prohibitive. We show that under certain conditions, incorporation of a penalty terms in the objective can remedy inexact relaxations and lead to feasible points for non-convex QCQPs.

1.1 Contributions

This paper is concerned with non-convex quadratically-constrained quadratic programs for which SDP relaxations are inexact. In order to recover feasible points for QCQP, we incorporate a linear penalty term into the objective of SDP relaxations and show that feasible and near-globally optimal points can be obtained for the original QCQP by solving the resulting penalized SDPs. The penalty term is based on an arbitrary initial point. Our first result states that if the initial point is feasible and satisfies the linear independence constraint qualifica-

tion (LICQ) condition, then penalized SDP produces a unique solution that is feasible for the original QCQP and its objective value is not worse than that of the initial point. Our second result states that if the initial point is infeasible, but instead is sufficiently close to the feasible set and satisfies a generalized LICQ condition, then the unique optimal solution to penalized SDP is feasible for QCQP. Lastly, motivated by these results on constructing feasible points, we propose a heuristic sequential procedure for non-convex QCQP and demonstrate its performance on benchmark instances from the QPLIB library [29] as well as on large-scale system identification problems.

The success of sequential frameworks and penalized SDP in solving bilinear matrix inequalities (BMIs) is demonstrated in [36,38,40]. In [5], it is shown that penalized SDP is able to find the roots of overdetermined systems of polynomial equations. Moreover, the incorporation of penalty terms into the objective of SDP relaxations are proven to be effective for solving non-convex optimization problems in power systems [53,54,84,85]. These papers show that penalizing certain physical quantities in power network optimization problems such as reactive power loss or thermal loss facilitates the recovery of feasible points from convex relaxations. In [36], a sequential framework is introduced for solving BMIs without theoretical guarantees. Papers [38,40] investigate this approach further and offer theoretical results through the notion of generalized Mangasarian–Fromovitz regularity condition. However, these conditions are not valid in the presence of equality constraints and for general QCQPs. Motivated by the success of penalized SDP, this paper offers a theoretical framework for general QCQP and, by extension, polynomial optimization problems.

1.2 Notations

Throughout the paper, scalars, vectors, and matrices are respectively shown by italic letters, lower-case italic bold letters, and upper-case italic bold letters. The symbols $\mathbb{R}$, $\mathbb{R}^n$, and $\mathbb{R}^{n \times m}$ denote the sets of real scalars, real vectors of size n, and real matrices of size $n \times m$, respectively. The set of $n \times n$ real symmetric matrices is shown by $\mathbb{S}_n$. For a given vector $\boldsymbol{a}$ and a matrix $\boldsymbol{A}$, the symbols a_i and A_{ij} respectively indicate the ith element of $\boldsymbol{a}$ and the (i, j)th element of $\boldsymbol{A}$. The symbols $\langle \cdot, \cdot \rangle$ and $\| \cdot \|_F$ denote the Frobenius inner product and norm of matrices, respectively. The notation $| \cdot |$ represents either the absolute value operator or cardinality of a set, depending on the context. The notation $\| \cdot \|_2$ denotes the ℓ_2 norm of vectors, matrices, and matrix pencils. The $n \times n$ identity matrix is denoted by $\boldsymbol{I}_n$. The origin of $\mathbb{R}^n$ is denoted by $\boldsymbol{0}_n$. The superscript $(\cdot)^\top$ and the symbol $\text{tr}\{\cdot\}$ represent the transpose and trace operators, respectively. Given a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, the notation $\sigma_{\min}(\boldsymbol{A})$ represents the minimum singular value of $\boldsymbol{A}$. The notation $\boldsymbol{A} \succeq 0$ means that $\boldsymbol{A}$ is symmetric positive-semidefinite. For a pair of $n \times n$ symmetric matrices $(\boldsymbol{A}, \boldsymbol{B})$ and proper cone $\mathcal{C} \subseteq \mathbb{S}_n$, the notation $\boldsymbol{A} \succeq_{\mathcal{C}} \boldsymbol{B}$ means that $\boldsymbol{A} - \boldsymbol{B} \in \mathcal{C}$, whereas $\boldsymbol{A} \succ_{\mathcal{C}} \boldsymbol{B}$ means that $\boldsymbol{A} - \boldsymbol{B}$ belongs to the interior of $\mathcal{C}$. Given an integer $r > 1$, define $\mathcal{C}_r$ as the cone of $n \times n$ symmetric matrices whose $r \times r$ principal submatrices are all positive semidefinite. Similarly, define $\mathcal{C}_r^*$ as the dual cone of $\mathcal{C}_r$, i.e., the cone of $n \times n$ symmetric matrices whose every $r \times r$ principal submatrix is positive semidefinite (i.e., factor-width bounded by r). Given a matrix $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and two sets of positive integers $\mathcal{S}_1$ and $\mathcal{S}_2$, define $\boldsymbol{A}\{\mathcal{S}_1, \mathcal{S}_2\}$ as the submatrix of $\boldsymbol{A}$ obtained by removing all rows of $\boldsymbol{A}$ whose indices do not belong to $\mathcal{S}_1$, and all columns of $\boldsymbol{A}$ whose indices do not belong to $\mathcal{S}_2$. Moreover, define $\boldsymbol{A}\{\mathcal{S}_1\}$ as the submatrix of $\boldsymbol{A}$ obtained by removing all rows of $\boldsymbol{A}$ that do not belong to $\mathcal{S}_1$. Given a vector $\boldsymbol{a} \in \mathbb{R}^n$ and a set $\mathcal{F} \subseteq \mathbb{R}^n$, define $d_{\mathcal{F}}(\boldsymbol{a})$ as the minimum distance between $\boldsymbol{a}$ and members of $\mathcal{F}$. Given a pair of integers (n, r), the binomial coefficient "n choose r" is denoted by $\binom{n}{r}$. The notations $\nabla_{\boldsymbol{x}} f(\boldsymbol{a})$ and

$\nabla_x^2 f(\boldsymbol{a})$, respectively, represent the gradient and Hessian of the function f, with respect to the vector $\boldsymbol{x}$, at a point $\boldsymbol{a}$.

1.3 Outline

The remainder of the paper is organized as follows. In Sect. 2, we review the basic lifted and reformulation linearization technique (RLT) as well as the standard SDP relaxations. Section 3 presents the main results of the paper: the penalized SDP, its theoretical analysis on producing a feasible solution along with a generalized linear independence constraint qualification, and finally the sequential penalization procedure. In Sect. 4 we present numerical experiments to test the effectiveness of the sequential penalization approach for non-convex QCQPs from the library of quadratic programming instances (QPLIB) as well as large-scale system identification problems. Finally, we conclude in Sect. 5 with a few final remarks.

2 Preliminaries

In this section, we review the lifting and reformulation-linearization technique (RLT) as well as the standard convex relaxations of QCQP that are necessary for the development of the main results on penalized SDP in Sect. 3. Consider a general quadratically-constrained quadratic program (QCQP):

$$\underset{\boldsymbol{x}\in\mathbb{R}^n}{\text{minimize}} \quad q_0(\boldsymbol{x}) \tag{1a}$$

$$\text{s.t.} \quad q_k(\boldsymbol{x}) \leq 0, \quad k \in \mathcal{I} \tag{1b}$$

$$q_k(\boldsymbol{x}) = 0, \quad k \in \mathcal{E}, \tag{1c}$$

where $\mathcal{I}$ and $\mathcal{E}$ index the sets of inequality and equality constraints, respectively. For every $k \in \{0\}\cup\mathcal{I}\cup\mathcal{E}$, $q_k\colon\mathbb{R}^n \to \mathbb{R}$ is a quadratic function of the form $q_k(\boldsymbol{x}) \triangleq \boldsymbol{x}^\top A_k\boldsymbol{x}+2\boldsymbol{b}_k^\top\boldsymbol{x}+c_k$, where $A_k \in \mathbb{S}_n$, $\boldsymbol{b}_k \in \mathbb{R}^n$, and $c_k \in \mathbb{R}$. Denote $\mathcal{F}$ as the feasible set of the QCQP (1a)–(1c). To derive the optimality conditions for a given point, it is useful to define the Jacobian matrix of the constraint functions.

Definition 1 (*Jacobian Matrix*) For every $\hat{\boldsymbol{x}} \in \mathbb{R}^n$, the Jacobian matrix $\mathcal{J}(\hat{\boldsymbol{x}})$ for the constraint functions $\{q_k\}_{k\in\mathcal{I}\cup\mathcal{E}}$ is

$$\mathcal{J}(\hat{\boldsymbol{x}}) \triangleq [\nabla_x q_1(\hat{\boldsymbol{x}}), \ldots, \nabla_x q_{|\mathcal{I}\cup\mathcal{E}|}(\hat{\boldsymbol{x}})]^\top. \tag{2}$$

For every $\mathcal{Q} \subseteq \mathcal{I} \cup \mathcal{E}$, define $\mathcal{J}_\mathcal{Q}(\hat{\boldsymbol{x}})$ as the submatrix of $\mathcal{J}(\hat{\boldsymbol{x}})$ resulting from the rows that belong to $\mathcal{Q}$.

Given a feasible point for the QCQP (1a)–(1c), the well-known linear independence constraint qualification (LICQ) condition can be used as a regularity criterion.

Definition 2 (*LICQ Condition*) A feasible point $\hat{\boldsymbol{x}} \in \mathcal{F}$ is LICQ regular if the rows of $\mathcal{J}_{\hat{\mathcal{B}}}(\hat{\boldsymbol{x}})$ are linearly independent, where $\hat{\mathcal{B}} \triangleq \{k \in \mathcal{I} \cup \mathcal{E} \mid q_k(\hat{\boldsymbol{x}}) = 0\}$ denotes the set of binding constraints at $\hat{\boldsymbol{x}}$.

Finding a feasible point for the QCQP (1a)–(1c), however, is NP-hard as the Boolean Satisfiability Problem (SAT) is a special case. Therefore, in Sect. 3, we introduce the notion of generalized LICQ as a regularity condition for both feasible and infeasible points.

2.1 Convex relaxation

A common approach for tackling the non-convex QCQP (1a)–(1c) introduces an auxiliary variable $X \in \mathbb{S}_n$ accounting for $xx^\top$. Then, the objective function (1a) and constraints (1b)–(1c) can be written as linear functions of x and X. For every $k \in \{0\} \cup \mathcal{I} \cup \mathcal{E}$, define $\bar{q}_k : \mathbb{R}^n \times \mathbb{S}_n \to \mathbb{R}$ as

$$\bar{q}_k(x, X) \triangleq \langle A_k, X \rangle + 2b_k^\top x + c_k. \tag{3}$$

Consider the following relaxation of QCQP (1a)–(1c):

$$\underset{x \in \mathbb{R}^n, X \in \mathbb{S}_n}{\text{minimize}} \quad \bar{q}_0(x, X) \tag{4a}$$

$$\text{s.t.} \quad \bar{q}_k(x, X) \le 0, \qquad k \in \mathcal{I} \tag{4b}$$

$$\bar{q}_k(x, X) = 0, \qquad k \in \mathcal{E} \tag{4c}$$

$$X - xx^\top \succeq_{\mathcal{C}_r} 0 \tag{4d}$$

where the additional conic constraint (4d) is a convex relaxation of the equation $X = xx^\top$. We refer to the convex problem (4a)–(4d) as the $r \times r$ SDP relaxation of the QCQP (1a)–(1c). The choice $r = n$ yields the well-known semidefinite programming (SDP) relaxation. Additionally, in the homogeneous case (i.e., if $b_0 = b_1 = \cdots = b_{|\mathcal{I} \cup \mathcal{E}|} = 0$), the case $r = 2$ leads to the second-order conic programming (SOCP) relaxation.

In the presence of affine constraints, the RLT method of Sherali and Adams [72] can be used to produce additional inequalities with respect to x and X to strengthen convex relaxations. This is covered in "Appendix B".

If the relaxed problem (4a)–(4d) has an optimal solution $\overset{*}{x}$ ($\overset{*}{x}, \overset{*}{X}$) that satisfies $\overset{*}{X} = \overset{*}{x}\overset{*}{x}^\top$, then the relaxation is said to be *exact* and $\overset{*}{x}$ is a globally optimal solution for the QCQP (1a)–(1c). The next section offers a penalization method for addressing the case where relaxations are not exact.

3 Penalized SDP

If the relaxed problem (4a)–(4d) is not exact, the resulting solution is not necessarily feasible for the original QCQP (1a)–(1c). In this case, we use an initial point $\hat{x} \in \mathbb{R}^n$ (either feasible or infeasible) to revise the objective function, resulting in a *penalized SDP* of the form:

$$\underset{x \in \mathbb{R}^n, X \in \mathbb{S}_n}{\text{minimize}} \quad \bar{q}_0(x, X) + \eta \times (\text{tr}\{X\} - 2\hat{x}^\top x + \hat{x}^\top \hat{x}) \tag{5a}$$

$$\text{s.t.} \quad \bar{q}_k(x, X) \le 0, \qquad k \in \mathcal{I} \tag{5b}$$

$$\bar{q}_k(x, X) = 0, \qquad k \in \mathcal{E} \tag{5c}$$

$$X - xx^\top \succeq_{\mathcal{C}_r} 0 \tag{5d}$$

where $\eta > 0$ is a fixed penalty parameter. Note that the penalty term $\text{tr}\{X\} - 2\hat{x}^\top x + \hat{x}^\top \hat{x}$ equals zero for $X = \hat{x}\hat{x}^\top$. The penalization is said to be *tight* if problem (5a)–(5d) has a unique optimal solution $(\overset{*}{x}, \overset{*}{X})$ that satisfies $\overset{*}{X} = \overset{*}{x}\overset{*}{x}^\top$. In the next section, we give sufficient conditions under which penalized SDP is tight.

3.1 Theoretical analysis

The following theorem guarantees that if $\hat{x}$ is feasible and satisfies the LICQ regularity condition (in Sect. 2), then the solution of (5a)–(5d) is guaranteed to be feasible for the QCQP (1a)–(1c) for an appropriate choice of η.

Theorem 1 *Let $\hat{x}$ be a feasible point for the QCQP (1a)–(1b) that satisfies the LICQ condition. For sufficiently large $\eta > 0$, the SDP (5a)–(5d) has a unique optimal solution $(\overset{*}{x}, \overset{*}{X})$ such that $\overset{*}{X} = \overset{*}{x}\overset{*}{x}^\top$. Moreover, $\overset{*}{x}$ is feasible for (1a)–(1c) and satisfies $q_0(\overset{*}{x}) \leq q_0(\hat{x})$.*

Proof The proof is given in Sect. 3.2. $\square$

If $\hat{x}$ is not feasible, but satisfies a generalized LICQ regularity condition, introduced below, and is close enough to the feasible set $\mathcal{F}$, then the penalization is still tight for large enough $\eta > 0$. This result is described formally in Theorem 2. First, we define a distance measure from an arbitrary point in $\mathbb{R}^n$ to the feasible set of the problem.

Definition 3 (*Distance Function*) The distance function $d_{\mathcal{F}} : \mathbb{R}^n \to \mathbb{R}$ is defined as

$$d_{\mathcal{F}}(\hat{x}) \triangleq \min\{\|x - \hat{x}\|_2 \mid x \in \mathcal{F}\}. \tag{6}$$

Definition 4 (*Generalized LICQ Condition*) For every $\hat{x} \in \mathbb{R}^n$, the set of *quasi-binding* constraints is defined as

$$\hat{\mathcal{B}} \triangleq \mathcal{E} \cup \left\{ k \in \mathcal{I} \;\middle|\; q_k(\hat{x}) + \|\nabla q_k(\hat{x})\|_2 d_{\mathcal{F}}(\hat{x}) + \frac{\|\nabla^2 q_k(\hat{x})\|_2}{2} d_{\mathcal{F}}(\hat{x})^2 \geq 0 \right\}. \tag{7}$$

The point $\hat{x}$ is said to satisfy the GLICQ condition if the rows of $\mathcal{J}_{\hat{\mathcal{B}}}(\hat{x})$ are linearly independent. Moreover, the sensitivity function $s : \mathbb{R}^n \to \mathbb{R}$ is defined as

$$s(\hat{x}) \triangleq \begin{cases} \sigma_{\min}(\mathcal{J}_{\hat{\mathcal{B}}}(\hat{x})) & \text{if } \hat{x} \text{ satisfies GLICQ} \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

where $\sigma_{\min}(\mathcal{J}_{\hat{\mathcal{B}}}(\hat{x}))$ denotes the smallest singular value of $\mathcal{J}_{\hat{\mathcal{B}}}(\hat{x})$.

Observe that if $\hat{x}$ is feasible, then $d_{\mathcal{F}}(\hat{x}) = 0$, and GLICQ condition reduces to the LICQ condition. Moreover, GLICQ is satisfied if and only if $s(\hat{x}) > 0$.

The next definition introduces the notion of matrix pencil corresponding to the QCQP (1a)–(1c), which will be used as a sensitivity measure.

Definition 5 (*Pencil Norm*) For the QCQP (1a)–(1c), define the corresponding matrix pencil $P : \mathbb{R}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|} \to \mathbb{S}_n$ as follows:

$$P(\gamma, \mu) \triangleq \sum_{k \in \mathcal{I}} \gamma_k A_k + \sum_{k \in \mathcal{E}} \mu_k A_k. \tag{9}$$

Moreover, define the pencil norm $\|P\|_2$ as

$$\|P\|_2 \triangleq \max\left\{ \|P(\gamma, \mu)\|_2 \mid \|\gamma\|_2^2 + \|\mu\|_2^2 = 1 \right\}, \tag{10}$$

which is upperbounded by $\sqrt{\sum_{k \in \mathcal{I} \cup \mathcal{E}} \|A_k\|_2^2}$.

Theorem 2 *Let $\hat{x} \in \mathbb{R}^n$ satisfy the GLICQ condition for the QCQP (1a)–(1b), and assume that*

$$d_{\mathcal{F}}(\hat{x}) < \left[1 + \binom{n-1}{r-1}\right]^{-1} \frac{s(\hat{x})}{2\|P\|_2}, \tag{11}$$

where $\binom{n-1}{r-1}$ denotes the binomial coefficient "$n-1$ choose $r-1$" and the distance function $d_{\mathcal{F}}(\cdot)$, sensitivity function $s(\cdot)$ and pencil norm $\|P\|_2$ are given by Definitions 3, 4 and 5, respectively.

If η is sufficiently large, then the convex problem (5a)–(5d) has a unique optimal solution $(\overset{*}{x}, \overset{*}{X})$ such that $\overset{*}{X} = \overset{*}{x}\overset{*}{x}^\top$ and $\overset{*}{x}$ is feasible for (1a)–(1c).

Proof The proof is given in Sect. 3.2. □

The motivation behind Theorem 2 is to show that even an infeasible initial point can be used to produce feasible points. It should be noted that, in general, it is computationally hard to calculate the exact distance from $\mathcal{F}$ and to verify GLICQ as a consequence. However, local search methods can be used in practice to find a local solution for (6), resulting in upper bounds on feasibility distance. In Sect. 4, we use this simple technique to verify condition (11) for several benchmark cases. It should be noted that despite the theoretical insights offered by Theorems 1 and 2, they do not provide any practical bounds for η. Additionally, this section is primarily focused on offering a non-constructive proof for the existence of η and we leave the derivation of analytical bounds for future work. In Sect. 4, we demonstrate that for real-world problems, appropriate choices of η can be found via a simple bisection technique.

3.2 Proof of the theorems

The rest of this section is devoted to proving Theorems 1 and 2. To this end, it is convenient to consider the following optimization problem:

$$\underset{x \in \mathbb{R}^n}{\text{minimize}} \quad q_0(x) + \eta\|x - \hat{x}\|_2^2 \tag{12a}$$

$$\text{s.t.} \quad q_k(x) \leq 0, \quad k \in \mathcal{I} \tag{12b}$$

$$q_k(x) = 0, \quad k \in \mathcal{E}. \tag{12c}$$

Observe that the problem (5a)–(5d) is a convex relaxation of (12a)–(12c) and this is the motivation behind its introduction.

Consider an $\alpha > 0$ for which the inequality

$$|q_0(x)| \leq \alpha\|x - \hat{x}\|_2^2 + \alpha, \tag{13}$$

is satisfied for every $x \in \mathbb{R}^n$. If $\eta > \alpha$, then the objective function (12a) is lower bounded by $-\alpha$. Hence, if $\mathcal{F}$ is non-empty, then the optimal solution of (12a)–(12c) is attainable, i.e., there exists $\overset{*}{x} \in \mathcal{F}$ which satisfies

$$q_0(\overset{*}{x}) \leq q_0(x)$$

for every $x \in \mathcal{F}$. To prove the existence of α, assume that

$$\alpha \geq \sigma_{\max}\left(\begin{bmatrix} A_0 & b_0 \\ b_0^\top & -\hat{x}^\top A_0 \hat{x} - 2b_0^\top \hat{x} \end{bmatrix}\right) \sigma_{\min}^{-1}\left(\begin{bmatrix} I_n & -\hat{x} \\ -\hat{x}^\top & \frac{1}{2} + \hat{x}^\top \hat{x} \end{bmatrix}\right) \tag{14a}$$

$$\alpha \geq 2|\hat{x}^\top A_0 \hat{x} + 2b_0^\top \hat{x} + c_0| \tag{14b}$$

then we have

$$|q_0(x)| = \left| \begin{bmatrix} x^\top & 1 \end{bmatrix} \begin{bmatrix} A_0 & b_0 \\ b_0^\top & -\hat{x}^\top A_0 \hat{x} - 2b_0^\top \hat{x} \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} + \hat{x}^\top A_0 \hat{x} + 2b_0^\top \hat{x} + c_0 \right| \tag{15a}$$

$$\leq \alpha \begin{bmatrix} x^\top & 1 \end{bmatrix} \begin{bmatrix} I_n & -\hat{x} \\ -\hat{x}^\top & \frac{1}{2} + \hat{x}^\top \hat{x} \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} + \frac{\alpha}{2} \tag{15b}$$

$$= \alpha \|x - \hat{x}\|_2^2 + \alpha \tag{15c}$$

which concludes (13).

The next lemma shows that by increasing the penalty term η, the optimal solution $\overset{*}{x}$ can get as close to the initial point $\hat{x}$ as $d_\mathcal{F}(\hat{x})$. This lemma will later be used to show that $\overset{*}{x}$ can inherit the LICQ property from $\hat{x}$.

Lemma 1 *Given an arbitrary $\hat{x} \in \mathbb{R}^n$ and $\varepsilon > 0$, for sufficiently large $\eta > 0$, every optimal solution $\overset{*}{x}$ of the problem (12a)–(12c) satisfies*

$$0 \leq \|\overset{*}{x} - \hat{x}\|_2 - d_\mathcal{F}(\hat{x}) \leq \varepsilon. \tag{16}$$

Proof Consider an optimal solution $\overset{*}{x}$. Due to Definition 3, the distance between $\hat{x}$ and every member of $\mathcal{F}$ is not less than $d_\mathcal{F}(\hat{x})$, which concludes the left side of (16). Let x_d be an arbitrary member of the set $\{x \in \mathcal{F} \mid \|x - \hat{x}\|_2 = d_\mathcal{F}(\hat{x})\}$. Due to the optimality of $\overset{*}{x}$, we have

$$q_0(\overset{*}{x}) + \eta \|\overset{*}{x} - \hat{x}\|_2^2 \leq q_0(x_d) + \eta \|x_d - \hat{x}\|_2^2. \tag{17}$$

According to the inequalities (17) and (13), one can write

$$(\eta - \alpha)\|\overset{*}{x} - \hat{x}\|_2^2 - \alpha \leq (\eta + \alpha)\|x_d - \hat{x}\|_2^2 + \alpha \tag{18a}$$

$$\Rightarrow \|\overset{*}{x} - \hat{x}\|_2^2 \leq \|x_d - \hat{x}\|_2^2 + \frac{2\alpha}{\eta - \alpha}(1 + \|x_d - \hat{x}\|_2^2) \tag{18b}$$

$$\Rightarrow \|\overset{*}{x} - \hat{x}\|_2^2 \leq d_\mathcal{F}(\hat{x})^2 + \frac{2\alpha}{\eta - \alpha}(1 + d_\mathcal{F}(\hat{x})^2), \tag{18c}$$

which concludes the right side of (16), provided that $\eta \geq \alpha + 2\alpha(1 + d_\mathcal{F}(\hat{x})^2)[\varepsilon^2 + 2\varepsilon d_\mathcal{F}(\hat{x})]^{-1}$. $\qquad\square$

Lemma 2 *Assume that $\hat{x} \in \mathbb{R}^n$ satisfies the GLICQ condition for the problem (12a)–(12c). Given an arbitrary $\varepsilon > 0$, for sufficiently large $\eta > 0$, every optimal solution $\overset{*}{x}$ of the problem satisfies*

$$s(\hat{x}) - s(\overset{*}{x}) \leq 2d_\mathcal{F}(\hat{x})\|P\|_2 + \varepsilon. \tag{19}$$

Proof Let $\hat{\mathcal{B}}$ and $\overset{*}{\mathcal{B}}$ denote the sets of quasi-binding constraints for $\hat{x}$ and binding constraints for $\overset{*}{x}$, respectively (based on Definition 4). Due to Lemma 1, for every $k \in \mathcal{I} \setminus \hat{\mathcal{B}}$ and every arbitrary $\varepsilon_1 > 0$, we have

$$q_k(\overset{*}{x}) - q_k(\hat{x}) = 2(A_k \hat{x} + b_k)^\top(\overset{*}{x} - \hat{x}) + (\overset{*}{x} - \hat{x})^\top A_k(\overset{*}{x} - \hat{x})$$

$$\leq \|\nabla q_k(\hat{x})\|_2 \|\overset{*}{x} - \hat{x}\|_2 + \|A_k\|_2 \|\overset{*}{x} - \hat{x}\|_2^2$$

$$\leq \|\nabla q_k(\hat{x})\|_2 d_\mathcal{F}(\hat{x}) + \|A_k\|_2 d_\mathcal{F}(\hat{x})^2 + \varepsilon_1 < -q_k(\hat{x}), \tag{20}$$

if η is sufficiently large, which yields $\overset{*}{\mathcal{B}} \subseteq \hat{\mathcal{B}}$. Let $\boldsymbol{v} \in \mathbb{R}^{|\hat{\mathcal{B}}|}$ be the left singular vector of $\mathcal{J}_{\hat{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})$, corresponding to the smallest singular value. Hence

$$s(\overset{*}{\boldsymbol{x}}) = \sigma_{\min}\{\mathcal{J}_{\overset{*}{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})\} \geq \sigma_{\min}\{\mathcal{J}_{\hat{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})\} = \|\mathcal{J}_{\hat{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})^{\top}\boldsymbol{v}\|_2 \tag{21a}$$

$$\geq \|\mathcal{J}_{\hat{\mathcal{B}}}(\hat{\boldsymbol{x}})^{\top}\boldsymbol{v}\|_2 - \|[\mathcal{J}_{\hat{\mathcal{B}}}(\hat{\boldsymbol{x}}) - \mathcal{J}_{\hat{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})]^{\top}\boldsymbol{v}\|_2 \tag{21b}$$

$$\geq \sigma_{\min}\{\mathcal{J}_{\hat{\mathcal{B}}}(\hat{\boldsymbol{x}})\}\|\boldsymbol{v}\|_2 - 2\|\boldsymbol{P}\|_2\|\hat{\boldsymbol{x}} - \overset{*}{\boldsymbol{x}}\|_2\|\boldsymbol{v}\|_2 \tag{21c}$$

$$\geq s(\hat{\boldsymbol{x}}) - 2\|\boldsymbol{P}\|_2\|\hat{\boldsymbol{x}} - \overset{*}{\boldsymbol{x}}\|_2 \tag{21d}$$

$$\geq s(\hat{\boldsymbol{x}}) - 2d_{\mathcal{F}}(\hat{\boldsymbol{x}})\|\boldsymbol{P}\|_2 - \varepsilon, \tag{21e}$$

if η is large, which concludes the inequality (19). $\qquad\square$

In light of Lemma 2, if $\hat{\boldsymbol{x}}$ is GLICQ regular and relatively close to $\mathcal{F}$, then $\overset{*}{\boldsymbol{x}}$ is LICQ regular as well. This will be used next to prove the existence of Lagrange multipliers.

Lemma 3 *Let $\overset{*}{\boldsymbol{x}}$ be an optimal solution of the problem* (12a)–(12c)*, and assume that $\overset{*}{\boldsymbol{x}}$ is LICQ regular. There exists a pair of dual vectors $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_{+}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$ that satisfies the following Karush–Kuhn–Tucker (KKT) conditions:*

$$2(\eta\boldsymbol{I} + \boldsymbol{A}_0)(\overset{*}{\boldsymbol{x}} - \hat{\boldsymbol{x}}) + 2(\boldsymbol{A}_0\hat{\boldsymbol{x}} + \boldsymbol{b}_0) + \mathcal{J}(\overset{*}{\boldsymbol{x}})^{\top}[\overset{*}{\boldsymbol{\gamma}}^{\top}, \overset{*}{\boldsymbol{\mu}}^{\top}]^{\top} = 0, \tag{22a}$$

$$\overset{*}{\gamma}_k q_k(\overset{*}{\boldsymbol{x}}) = 0, \qquad \forall k \in \mathcal{I}. \tag{22b}$$

Proof Due to the LICQ condition, there exists a pair of dual vectors $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_{+}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$, which satisfies the KKT stationarity and complementary slackness conditions. Due to stationarity, we have

$$\begin{aligned}
0 &= \nabla_{\boldsymbol{x}}\mathcal{L}(\overset{*}{\boldsymbol{x}}, \overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}})/2 \\
&= \eta(\overset{*}{\boldsymbol{x}} - \hat{\boldsymbol{x}}) + (\boldsymbol{A}_0\overset{*}{\boldsymbol{x}} + \boldsymbol{b}_0) + \boldsymbol{P}(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}})\overset{*}{\boldsymbol{x}} + \sum_{k\in\mathcal{I}}\overset{*}{\gamma}_k\boldsymbol{b}_k + \sum_{k\in\mathcal{E}}\overset{*}{\mu}_k\boldsymbol{b}_k \\
&= (\eta\boldsymbol{I} + \boldsymbol{A}_0)(\overset{*}{\boldsymbol{x}} - \hat{\boldsymbol{x}}) + (\boldsymbol{A}_0\hat{\boldsymbol{x}} + \boldsymbol{b}_0) + \mathcal{J}(\overset{*}{\boldsymbol{x}})^{\top}[\overset{*}{\boldsymbol{\gamma}}^{\top}, \overset{*}{\boldsymbol{\mu}}^{\top}]^{\top}/2. \tag{23}
\end{aligned}$$

Moreover, (22b) is concluded from the complementary slackness. $\qquad\square$

The next lemma bounds the Lagrange multipliers whose existence is proven previously. This bound is helpful to prove that $\overset{*}{\boldsymbol{X}} = \overset{*}{\boldsymbol{x}}\overset{*}{\boldsymbol{x}}^{\top}$.

Lemma 4 *Consider an arbitrary $\varepsilon > 0$ and suppose $\hat{\boldsymbol{x}} \in \mathbb{R}^n$ satisfies the inequality*

$$s(\hat{\boldsymbol{x}}) > 2d_{\mathcal{F}}(\hat{\boldsymbol{x}})\|\boldsymbol{P}\|_2. \tag{24}$$

If η is sufficiently large, for every optimal solution $\overset{*}{\boldsymbol{x}}$ of the problem (12a)–(12c)*, there exists a pair of dual vectors $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_{+}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$ that satisfies the inequality*

$$\frac{1}{\eta}\sqrt{\|\overset{*}{\boldsymbol{\gamma}}\|_2^2 + \|\overset{*}{\boldsymbol{\mu}}\|_2^2} \leq \frac{2d_{\mathcal{F}}(\hat{\boldsymbol{x}})}{s(\hat{\boldsymbol{x}}) - 2d_{\mathcal{F}}(\hat{\boldsymbol{x}})\|\boldsymbol{P}\|_2} + \varepsilon \tag{25}$$

as well as the Eqs. (22a) *and* (22b)*.*

Proof Due to Lemma 3, there exists $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_{+}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$ that satisfies the Eqs. (22a) and (22b). Let $\boldsymbol{\tau} \triangleq [\overset{*}{\boldsymbol{\gamma}}^{\top}, \overset{*}{\boldsymbol{\mu}}^{\top}]^{\top}$ and let $\overset{*}{\mathcal{B}}$ be the set of binding constraints for $\overset{*}{\boldsymbol{x}}$. Due to Eqs. (22a) and (22b), one can write

$$2(\eta\boldsymbol{I} + \boldsymbol{A}_0)(\overset{*}{\boldsymbol{x}} - \hat{\boldsymbol{x}}) + 2(\boldsymbol{A}_0\hat{\boldsymbol{x}} + \boldsymbol{b}_0) + \mathcal{J}_{\overset{*}{\mathcal{B}}}(\overset{*}{\boldsymbol{x}})^{\top}\boldsymbol{\tau}\{\overset{*}{\mathcal{B}}\} = 0. \tag{26}$$

Let $\phi \triangleq s(\hat{x}) - 2d_{\mathcal{F}}(\hat{x})\|P\|_2$ and define

$$\varepsilon_1 \triangleq \phi \times \frac{\varepsilon - 2\eta^{-1}\phi^{-1}(\|A_0\hat{x} + b_0\|_2 + d_{\mathcal{F}}(\hat{x})\|A_0\|_2)}{\varepsilon + 2 + 2\eta^{-1}\|A_0\|_2 + 2\phi^{-1}d_{\mathcal{F}}(\hat{x})}. \tag{27}$$

If η is sufficiently large, ε_1 is positive and based on Lemmas 1 and 2, we have

$$
\begin{aligned}
\frac{\|\boldsymbol{\tau}\|_2}{\eta} = \frac{\|\boldsymbol{\tau}\{\overset{*}{\mathcal{B}}\}\|_2}{\eta} &\leq \frac{2\|(\eta I + A_0)(\overset{*}{x} - \hat{x}) + (A_0\hat{x} + b_0)\|_2}{\eta\sigma_{\min}\{\mathcal{J}_{\overset{*}{\mathcal{B}}}(\overset{*}{x})\}} \\
&\leq \frac{2\eta\|\overset{*}{x} - \hat{x}\|_2 + 2\|A_0\|_2\|\overset{*}{x} - \hat{x}\|_2 + 2\|A_0\hat{x} + b_0\|_2}{\eta s(\overset{*}{x})} \\
&\leq \frac{2(d_{\mathcal{F}}(\hat{x}) + \varepsilon_1) + 2\eta^{-1}[\|A_0\|_2(d_{\mathcal{F}}(\hat{x}) + \varepsilon_1) + \|A_0\hat{x} + b_0\|_2]}{s(\hat{x}) - 2d_{\mathcal{F}}(\hat{x})\|P\|_2 - \varepsilon_1} \\
&= \frac{2d_{\mathcal{F}}(\hat{x})}{s(\hat{x}) - 2d_{\mathcal{F}}(\hat{x})\|P\|_2} + \varepsilon,
\end{aligned}
\tag{28}
$$

where the last equality is a result of the Eq. (27). □

The next two lemmas provide sufficient conditions for $\overset{*}{X} = \overset{*}{x}\overset{*}{x}^\top$ with respect to Lagrange multipliers that will be used later to prove Theorems 1 and 2.

Lemma 5 *Consider an optimal solution $\overset{*}{x}$ of the problem (12a)–(12c), and a pair of dual vectors $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_+^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$ that satisfies the conditions (22a) and (22b). If the matrix inequality*

$$\eta I + A_0 + P(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \succ_{\mathcal{D}_r} 0, \tag{29}$$

holds true, then the pair $(\overset{*}{x}, \overset{*}{x}\overset{*}{x}^\top)$ is the unique primal solution to the penalized SDP (5a)–(5d).

Proof Let $\boldsymbol{\Lambda} \in \mathbb{S}_n^+$ denotes the dual variable associated with the conic constraint (5d). Then, the KKT conditions for the problem (5a)–(5d) can be written as follows:

$$\nabla_x \bar{\mathcal{L}}(x, X, \boldsymbol{\gamma}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = 2\left(\boldsymbol{\Lambda}x - \eta\hat{x} + b_0 + \sum_{k \in \mathcal{I}} \overset{*}{\gamma}_k b_k + \sum_{k \in \mathcal{E}} \overset{*}{\mu}_k b_k\right) = 0, \tag{30a}$$

$$\nabla_X \bar{\mathcal{L}}(x, X, \boldsymbol{\gamma}, \boldsymbol{\mu}, \boldsymbol{\Lambda}) = \eta I + A_0 + P(\boldsymbol{\gamma}, \boldsymbol{\mu}) - \boldsymbol{\Lambda} = 0, \tag{30b}$$

$$\gamma_k q_k(x) = 0, \quad \forall k \in \mathcal{I} \tag{30c}$$

$$\langle \boldsymbol{\Lambda}, xx^\top - X \rangle = 0, \tag{30d}$$

where $\bar{\mathcal{L}} : \mathbb{R}^n \times \mathbb{S}_n \times \mathbb{R}^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|} \times \mathbb{S}_n \to \mathbb{R}$ is the Lagrangian function, Eqs. (30a) and (30b) account for stationarity with respect to x and X, respectively, and Eqs. (30c) and (30d) are the complementary slackness conditions for the constraints (5b) and (5d), respectively. Define

$$\overset{*}{\boldsymbol{\Lambda}} \triangleq \eta I + A_0 + P(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}). \tag{31}$$

Due to Lemma 3, if η is sufficiently large, $\overset{*}{x}$ and $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}})$ satisfy the Eqs. (22a) and (22b), which yield the optimality conditions (30a)–(30d), if $x = \overset{*}{x}, X = \overset{*}{x}\overset{*}{x}^\top, \boldsymbol{\gamma} = \overset{*}{\boldsymbol{\gamma}}, \boldsymbol{\mu} = \overset{*}{\boldsymbol{\mu}}$, and $\boldsymbol{\Lambda} = \overset{*}{\boldsymbol{\Lambda}}$. Therefore, the pair $(\overset{*}{x}, \overset{*}{x}\overset{*}{x}^\top)$ is a primal optimal points for the penalized SDP (5a)–(5d). Note that due to positive semidefiniteness of $\overset{*}{\boldsymbol{\Lambda}}$, the condition (30d) implies $xx^\top - X = 0$.

Since the KKT conditions hold for every pair of primal and dual solutions, we have

$$\overset{*}{\boldsymbol{x}} = \overset{*}{\boldsymbol{\Lambda}}^{-1} \left(\eta \hat{\boldsymbol{x}} - \boldsymbol{b}_0 - \sum_{k \in \mathcal{I}} \overset{*}{\gamma}_k \boldsymbol{b}_k - \sum_{k \in \mathcal{E}} \overset{*}{\mu}_k \boldsymbol{b}_k \right) \tag{32}$$

and $\overset{*}{X} = \overset{*}{\boldsymbol{x}} \overset{*}{\boldsymbol{x}}^\top$, according to the Eqs. (30a) and (30d), respectively, which implies the uniqueness of the solution. □

Lemma 6 *Consider an optimal solution $\overset{*}{\boldsymbol{x}}$ of the problem* (12a)–(12c), *and a pair of dual vectors* $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}) \in \mathbb{R}_+^{|\mathcal{I}|} \times \mathbb{R}^{|\mathcal{E}|}$ *that satisfies the conditions* (22a) *and* (22b). *If the inequality,*

$$\frac{1}{\eta} \sqrt{\|\overset{*}{\boldsymbol{\gamma}}\|_2^2 + \|\overset{*}{\boldsymbol{\mu}}\|_2^2} < \binom{n-1}{r-1}^{-1} \frac{1}{\|\boldsymbol{P}\|_2} - \frac{\|\boldsymbol{A}_0\|_2}{\eta \|\boldsymbol{P}\|_2} \tag{33}$$

holds true, then the pair $(\overset{*}{\boldsymbol{x}}, \overset{*}{\boldsymbol{x}} \overset{*}{\boldsymbol{x}}^\top)$ is the unique primal solution to the penalized SDP (5a)–(5d).

Proof Based on Lemma 5, it suffices to prove the conic inequality (29). Define

$$\boldsymbol{K} \triangleq \boldsymbol{A}_0 + \boldsymbol{P}(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}}). \tag{34}$$

It follows that

$$\|\boldsymbol{K}\|_2 \leq \|\boldsymbol{A}_0\|_2 + \sum_{k \in \mathcal{I}} \overset{*}{\gamma}_k \|\boldsymbol{A}_k\|_2 + \sum_{k \in \mathcal{E}} \overset{*}{\mu}_k \|\boldsymbol{A}_k\|_2, \tag{35a}$$

$$\leq \|\boldsymbol{A}_0\|_2 + \|\boldsymbol{P}\|_2 \sqrt{\|\overset{*}{\boldsymbol{\gamma}}\|_2^2 + \|\overset{*}{\boldsymbol{\mu}}\|_2^2} \,. \tag{35b}$$

Let $\mathcal{R}$ be the set of all r-member subsets of $\{1, 2, \ldots, n\}$. Hence,

$$\eta \boldsymbol{I} + \boldsymbol{K} = \sum_{\mathcal{K} \in \mathcal{R}} \boldsymbol{I}\{\mathcal{K}\}^\top \boldsymbol{R}_\mathcal{K} \, \boldsymbol{I}\{\mathcal{K}\}, \tag{36}$$

where

$$\boldsymbol{R}_\mathcal{K} = \binom{n-1}{r-1}^{-1} [\eta \boldsymbol{I}\{\mathcal{K}, \mathcal{K}\} + \boldsymbol{K}\{\mathcal{K}, \mathcal{K}\}]. \tag{37}$$

Due to the inequalities (33) and (35), we have $\boldsymbol{R}_\mathcal{K} \succ 0$ for every $\mathcal{K} \in \mathcal{R}$, which proves that $\eta \boldsymbol{I} + \boldsymbol{K} \succ_{\mathcal{D}_r} 0$. □

Proof of Theorem 2 Let $\overset{*}{\boldsymbol{x}}$ be an optimal solution of the problem (12a)–(12c). According to the assumption (11), the inequality (24) holds true, and due to Lemma 4, if η is sufficiently large, there exists a corresponding pair of dual vectors $(\overset{*}{\boldsymbol{\gamma}}, \overset{*}{\boldsymbol{\mu}})$ that satisfies the inequality (25). Now, according to the inequality (11), we have

$$\frac{2d_\mathcal{F}(\hat{\boldsymbol{x}})}{s(\hat{\boldsymbol{x}}) - 2d_\mathcal{F}(\hat{\boldsymbol{x}}) \|\boldsymbol{P}\|_2} \leq \frac{1}{\binom{n-1}{r-1} \|\boldsymbol{P}\|_2} \tag{38}$$

and therefore (25) concludes (33). Hence, according to Lemma 6, the pair $(\overset{*}{\boldsymbol{x}}, \overset{*}{\boldsymbol{x}} \overset{*}{\boldsymbol{x}}^\top)$ is the unique primal solution to the penalized SDP (5a)–(5d). □

Proof of Theorem 1 If $\hat{\boldsymbol{x}}$ is feasible, then $d_\mathcal{F}(\hat{\boldsymbol{x}}) = 0$. Therefore, the tightness of the penalization for Theorem 1 is a direct consequence of Theorem 2. Denote the unique optimal solution of the penalized SDP as $(\overset{*}{\boldsymbol{x}}, \overset{*}{\boldsymbol{x}} \overset{*}{\boldsymbol{x}}^\top)$. Then it is straightforward to verify the inequality $q_0(\overset{*}{\boldsymbol{x}}) \leq q_0(\hat{\boldsymbol{x}})$ by evaluating the objective function (5a) at the point $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{x}} \hat{\boldsymbol{x}}^\top)$. □

3.3 Sequential penalization procedure

In practice, the penalized SDP (5a)–(5d) can be initialized by a point that may not satisfy the conditions of Theorem 1 or Theorem 2 as these conditions are only sufficient, but not necessary. If the chosen initial point $\hat{x}$ does not result in a tight penalization, the penalized SDP (5a)–(5d) can be solved sequentially by updating the initial point until a feasible and near-optimal point is obtained. This heuristic procedure is described in Algorithm 1.

Algorithm 1 Sequential Penalized Conic Relaxation.

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initiate $\{q_k\}_{k \in \{0\} \cup \mathcal{I} \cup \mathcal{E}}$, $r \geq 2$, $\hat{x} \in \mathbb{R}^n$, and the fixed parameter $\eta > 0$
while stopping criterion is not met **do**
    solve the problem (5a)–(5d) with the initial point $\hat{x}$ to obtain $(\overset{*}{x}, \overset{*}{X})$
    set $\hat{x} \leftarrow \overset{*}{x}$
end while
return $\overset{*}{x}$

According to Theorem 2, once $\hat{x}$ is close enough to the feasible set $\mathcal{F}$, the penalization becomes tight, i.e., a feasible solution $\overset{*}{x}$ is recovered as the unique optimal solution to (5a)–(5d). Afterwards, in the subsequent iterations, according to Theorem 1, feasibility is preserved and the objective value does not increase. Note that Theorems 1 and 2 do not guarantee the existence of a global η that works for every member of the sequence generated by Algorithm 1. For this reason, we regard this procedure as a heuristic.

The following example illustrates the application of Algorithm 1 for a polynomial optimization.

Example 1 Consider the following three-dimensional polynomial optimization:

$$\underset{a,b,c \in \mathbb{R}}{\text{minimize}} \quad a \tag{39a}$$

$$\text{s.t.} \quad a^5 - b^4 - c^4 + 2a^3 + 2a^2b - 2ab^2 + 6abc - 2 = 0 \tag{39b}$$

To derive a QCQP reformulation of the problem (39a), (39b), we consider a variable $x \in \mathbb{R}^8$, whose elements account for the monomials a, b, c, a^2, b^2, c^2, ab, and a^3, respectively. This leads to the following QCQP:

$$\underset{x \in \mathbb{R}^8,}{\text{minimize}} \quad x_1 \tag{40a}$$

$$\text{s.t.} \quad x_4 x_8 - x_5^2 - x_6^2 + 2x_1 x_4 + 2x_2 x_4 - 2x_1 x_5 + 6x_3 x_7 - 2 = 0 \tag{40b}$$

$$x_4 - x_1^2 = 0 \tag{40c}$$

$$x_5 - x_2^2 = 0 \tag{40d}$$

$$x_6 - x_3^3 = 0 \tag{40e}$$

$$x_7 - x_1 x_2 = 0 \tag{40f}$$

$$x_8 - x_1 x_4 = 0 \tag{40g}$$

The transformation of the polynomial optimization to QCQP is standard and it is described in "Appendix A" for completeness. The global optimal objective value of the above QCQP equals -2.0198 and the lower-bound, offered by the standard SDP relaxation equals -89.8901. In order to solve the above QCQP, we run Algorithm 1, equipped with the SDP

relaxation (no additional valid inequalities) and penalty term $\eta = 0.025$. The trajectory with three different initializations $\hat{x}^1 = [0, 0, 0, 0, 0, 0, 0, 0]^\top$, $\hat{x}^2 = [-3, 0, 2, 9, 0, 4, 0, 27]^\top$, and $\hat{x}^3 = [0, 4, 0, 0, 16, 0, 0, 0]^\top$ are given in Table 1 and shown in Fig. 1. In all three cases, the algorithm achieves feasibility in 1–8 rounds. Moreover, a feasible solution with less than 0.2% gap from global optimality is attained within 10 rounds in all three cases. The example illustrates a case for which the heuristic Algorithm 1 is not sensitive to the choice of initial point.

4 Numerical experiments

In this section we describe numerical experiments to test the effectiveness of the sequential penalization method for non-convex QCQPs from the library of quadratic programming instances (QPLIB) [29] as well as large-scale system identification problems [25].

4.1 QPLIB problems

The experiments are performed on a desktop computer with a 12-core 3.0 GHz CPU and 256 GB RAM. MOSEK v8.1 [4] is used through MATLAB 2017a to solve the resulting SDPs. The size and number of constraints for each QPLIB instance are reported in Table 2.

4.1.1 Sequential penalization

Tables 3, 4, 5, and 6 report the results of Algorithm 1 for 2×2 SDP, 2×2 SDP + RLT, SDP, and SDP + RLT relaxations, respectively. The following valid inequalities are imposed on all of the convex relaxations:

$$X_{kk} - (x_k^{\text{lb}} + x_k^{\text{ub}})x_k + x_k^{\text{lb}}x_k^{\text{ub}} \leq 0, \qquad \forall k \in \{1, \ldots, n\} \qquad (41\text{a})$$

$$X_{kk} - (x_k^{\text{ub}} + x_k^{\text{ub}})x_k + x_k^{\text{ub}}x_k^{\text{ub}} \geq 0, \qquad \forall k \in \{1, \ldots, n\} \qquad (41\text{b})$$

$$X_{kk} - (x_k^{\text{lb}} + x_k^{\text{lb}})x_k + x_k^{\text{lb}}x_k^{\text{lb}} \geq 0, \qquad \forall k \in \{1, \ldots, n\} \qquad (41\text{c})$$

where $x^{\text{lb}}, x^{\text{ub}} \in \mathbb{R}^n$ are given lower and upper bounds on x. Problem (4a)–(4d) is solved with the following four settings:

- 2×2 *SDP relaxation* $r = 2$ and valid inequalities (41a)–(41c).
- 2×2 *SDP + RLT relaxation* $\mathcal{V} = \mathcal{H} \times \mathcal{H}$ and $r = 2$.
- *SDP relaxation* $r = n$ and valid inequalities (41a)–(41c).
- *SDP + RLT relaxation* $\mathcal{V} = \mathcal{H} \times \mathcal{H}$ and $r = n$,

where $\mathcal{V}$ and $\mathcal{H}$ is defined in "Appendix B". The assumption $\mathcal{V} = \mathcal{H} \times \mathcal{H}$ means that every pairs of linear constraints are used to generate RLT inequalities. Let $(\overset{*}{x}, \overset{*}{X})$ denote the optimal solution of the convex relaxation (4a)–(4d). We use the point $\hat{x} = \overset{*}{x}$ as the initial point of the algorithm.

The penalty parameter η is chosen via bisection as the smallest number of the form $\alpha \times 10^\beta$, which results in a tight penalization during the first six rounds, where $\alpha \in \{1, 2, 5\}$ and β is an integer. In all of the experiments, the value of η has remained static throughout Algorithm 1. Denote the sequence of penalized SDP solutions obtained by Algorithm 1 as

$$(x^{(1)}, X^{(1)}), \quad (x^{(2)}, X^{(2)}), \quad (x^{(3)}, X^{(3)}), \quad \ldots$$

Table 1 Trajectory of Algorithm 1 for three different initializations

| Round	$\hat{x}^1$				$\hat{x}^2$				$\hat{x}^3$			
	a (obj.)	b	c	$\mathrm{tr}\{\overset{*}{X}-\overset{*}{x}\overset{*}{x}{}^\top\}$	a (obj.)	b	c	$\mathrm{tr}\{\overset{*}{X}-\overset{*}{x}\overset{*}{x}{}^\top\}$	a (obj.)	b	c	$\mathrm{tr}\{\overset{*}{X}-\overset{*}{x}\overset{*}{x}{}^\top\}$
0	0.0000	0.0000	0.0000	–	−3.0000	0.0000	2.0000	–	0.0000	4.0000	0.0000	–
1	−1.2739	0.6601	−0.4697	2.1884	−2.5377	1.2831	−0.7380	138.9796	−1.5721	2.6848	−0.9492	39.2455
2	−1.5173	1.1445	−1.0128	$<10^{-11}$	−2.4389	2.0715	−1.3946	51.1170	−1.5749	2.7588	−1.3854	13.5140
3	−1.6882	1.3773	−1.2015	$<10^{-11}$	−2.2889	2.2685	−1.7098	23.0050	−1.6678	2.6583	−1.5228	0.9995
4	−1.8021	1.5739	−1.3561	$<10^{-11}$	−2.1878	2.3416	−1.8442	11.4963	−1.8322	2.6083	−1.5587	$<10^{-11}$
5	−1.8824	1.7447	−1.4873	$<10^{-11}$	−2.1194	2.3621	−1.9007	5.9206	−1.9460	2.5261	−1.6624	$<10^{-11}$
6	−1.9386	1.8930	−1.5992	$<10^{-11}$	−2.0733	2.3611	−1.9250	2.9082	−2.0002	2.4391	−1.7847	$<10^{-11}$
7	−1.9760	2.0180	−1.6923	$<10^{-11}$	−2.0423	2.3526	−1.9352	1.1594	−2.0156	2.3824	−1.8598	$<10^{-11}$
8	−1.9985	2.1175	−1.7656	$<10^{-11}$	−2.0214	2.3426	−1.9393	0.0938	−2.0189	2.3532	−1.8938	$<10^{-11}$
9	−2.0104	2.1907	−1.8193	$<10^{-11}$	−2.0197	2.3352	−1.9302	$<10^{-11}$	−2.0196	2.3387	−1.9079	$<10^{-11}$
10	−2.0160	2.2408	−1.8559	$<10^{-11}$	−2.0198	2.3304	−1.9240	$<10^{-11}$	−2.0197	2.3313	−1.9135	$<10^{-11}$
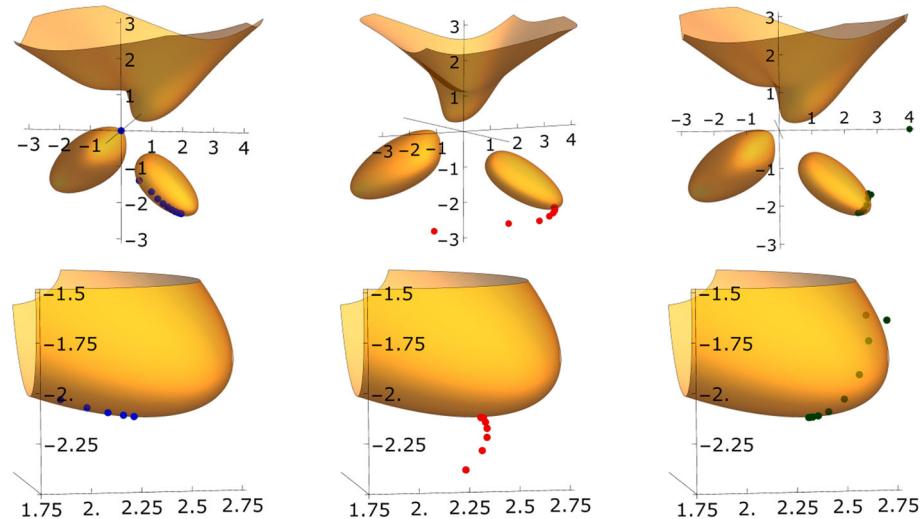
Fig. 1 Trajectory of Algorithm 1 for three different initializations. The yellow surface represents the feasible set and the blue, red and green points correspond to $\hat{x}^1$, $\hat{x}^2$ and $\hat{x}^3$, respectively. (Color figure online)

The smallest i such that

$$\text{tr}\{X^{(i)} - x^{(i)}(x^{(i)})^\top\} < 10^{-7} \tag{42}$$

is denoted by i^{feas}, i.e., it is the number of rounds that Algorithm 1 needs to attain a tight penalization.

Moreover, the smallest i such that

$$\frac{q_0(x^{(i-1)}) - q_0(x^{(i)})}{|q_0(x^{(i)})|} \leq 5 \times 10^{-4} \tag{43}$$

is denoted by i^{stop}, and $\text{UB} \triangleq q_0(x^{(i^{\text{stop}})})$. The following formula is used to calculate the final percentage gaps from the optimal costs reported by the QPLIB library:

$$\text{GAP}(\%) = 100 \times \frac{q_0^{\text{stop}} - q_0(x^{\text{QPLIB}})}{|q_0(x^{\text{QPLIB}})|}. \tag{44}$$

Moreover, $t(s)$ denotes the cumulative solver time in seconds for the i^{stop} rounds. Our results are compared with BARON [76] and COUENNE [10] by fixing the maximum solver times equal to the accumulative solver times spent by Algorithm 1. We ran BARON and COUENNE through GAMS v25.1.2 [30]. The resulting lower bounds, upper bounds and GAPs (from the Eq. (44)) are reported in Tables 3, 4, 5, and 6.

As demonstrated in the tables, penalized 2×2 SDP+RLT, SDP, and SDP+RLT have successfully obtained feasible points within 4% gaps from QPLIB solutions. Sequential SDP requires a smaller number of rounds compared to sequential 2×2 SDP to meet the stopping criterion (43). Using any of the relaxations, the infeasible initial points can be rounded to a feasible point with only two round of Algorithm 1 and all relaxations arrive at satisfactory gaps percentages. As demonstrated by the tables, the proposed sequential approach exhibits reasonable performance in comparison with the non-convex optimizers BARON and COUENNE.

Table 2 QPLIB benchmark problems

Inst	Total Var	Quad Cons	Total Cons	Inst	Total Var	Quad Cons	Total Cons	Inst	Total Var	Quad Cons	Total Cons	Inst	Total Var	Quad Cons	Total Cons
0343	50	0	1	1353	50	1	6	1535	60	60	66	1773	60	1	7
0911	50	50	50	1423	40	20	24	1619	50	25	30	1886	50	50	50
0975	50	10	10	1437	50	1	11	1661	60	1	13	1913	48	48	48
1055	40	20	20	1451	60	60	66	1675	60	1	13	1922	30	60	60
1143	40	20	24	1493	40	1	5	1703	60	30	36	1931	40	40	40
1157	40	1	9	1507	30	30	33	1745	50	50	55	1967	50	75	75

Table 3 Sequential penalized 2 × 2 SDP

Inst	Sequential penalized 2 × 2 SDP						BARON			COUENNE		
	η	i^{feas}	i^{stop}	t (s)	UB	GAP (%)	LB	UB	GAP (%)	LB	UB	GAP (%)
0343†	5e+2	1	100	75.27	−5.882	7.89	−95.372	−6.386	0.00	−7668.005	−6.386	0.00
0911	1e+1	1	29	22.91	−30.675	4.58	−172.777	0.000	100	−172.777	−31.026	3.49
0975	5e+0	6	18	46.36	−36.434	3.75	−47.428	−37.801	0.14	−171.113	−37.213	1.69
1055	1e+1	1	22	14.39	−32.620	1.26	−37.841	−33.037	0.00	−199.457	−33.037	0.00
1143	2e+1	1	44	25.68	−55.417	3.20	−69.522	−57.247	0.00	−384.45	−56.237	1.76
1157	2e+0	2	9	9.01	−10.938	0.10	−11.414	−10.948	0.00	−80.51	−10.948	0.00
1353	5e+0	1	48	84.90	−7.700	0.19	−7.925	−7.714	0.00	−73.28	−7.714	0.00
1423	5e+0	1	29	17.44	−14.684	1.90	−16.313	−14.968	0.00	−76.13	−14.871	0.65
1437	5e+0	1	36	54.57	−7.785	0.06	−9.601	−7.789	0.00	−87.58	−7.789	0.00
1451	2e+1	4	21	20.86	−85.598	2.26	−135.140	−87.577	0.00	−468.04	−86.860	0.82
1493	2e+1	1	18	14.49	−41.910	2.90	−47.239	−43.160	0.00	−395.69	−43.160	0.00
1507	2e+0	1	15	8.98	−8.289	0.15	−49.709	−8.301	0.00	−44.37	−8.301	0.00
1535	5e+0	1	26	28.16	−10.948	5.51	−13.407	−11.397	1.63	−107.86	−11.398	1.63
1619	5e+0	1	39	32.34	−9.210	0.08	−10.302	−9.217	0.00	−74.55	−9.217	0.00
1661	5e+0	1	32	87.50	−15.666	1.81	−19.667	−15.955	0.00	−139.25	−15.955	0.00
1675	2e+1	1	21	36.38	−75.485	0.24	−96.864	−75.669	0.00	−435.48	−75.669	0.00
1703	5e+1	2	30	31.82	−130.902	1.43	−180.935	−132.802	0.00	−929.92	−132.802	0.00
1745	2e+1	1	26	22.15	−71.704	0.93	−77.465	−72.377	0.00	−317.99	−72.377	0.00
1773	5e+0	1	56	148.79	−14.154	3.34	−21.581	−14.642	0.00	−118.65	−14.642	0.00
1886	2e+1	1	34	26.82	−78.604	0.09	−135.615	−78.672	0.00	−324.87	−78.672	0.00
1913	1e+1	1	28	21.91	−51.889	0.42	−68.555	−52.109	0.00	−164.26	−51.478	1.21
1922	1e+1	1	23	11.16	−35.437	1.43	−121.872	−35.951	0.00	−123.2	−35.951	0.00
1931	1e+1	1	13	8.78	−53.684	3.64	−85.196	−55.709	0.00	−204.08	−54.290	2.55
1967	5e+1	1	32	27.23	−105.570	1.87	−136.098	0.000	100	−622.57	−107.581	0.00
Max	500	6	100	148.79		7.89			100			3.34

Table 4 Sequential penalized 2 × 2 SDP + RLT

Inst	Sequential 2 × 2 SDP + RLT						BARON			COUENNE		
	η	i^{feas}	i^{stop}	t (s)	UB	GAP (%)	LB	UB	GAP (%)	LB	UB	GAP (%)
0343	1e+2	4	24	25.23	−5.945	6.91	−95.372	−6.386	0.00	−7668.005	−6.386	0.00
0911	1e+1	1	33	27.69	−30.923	3.81	−172.777	−32.148	0.00	−172.777	−31.026	3.49
0975	5e+0	6	15	4.10	−36.300	13.17	−47.428	−37.794	0.16	−171.113	−36.812	2.75
1055	1e+1	1	24	16.78	−32.666	1.12	−37.841	−33.037	0.00	−199.457	−33.037	0.00
1143	2e+1	1	30	32.66	−55.507	3.04	−69.522	−57.247	0.00	−384.45	−56.237	1.76
1157	2e+0	1	0	1.14	−10.948	0.00	−11.414	−10.948	0.00	−80.51	−10.948	0.00
1353	1e+0	3	11	19.41	−7.711	0.05	−7.925	−7.714	0.00	−73.28	−7.714	0.00
1423	2e+0	3	14	16.41	−14.730	1.59	−16.313	−14.968	0.00	−76.13	−14.871	0.65
1437	5e−1	4	8	21.62	−7.788	0.02	−9.601	−7.789	0.00	−87.58	−7.789	0.00
1451	2e+1	2	36	100.50	−87.502	0.09	−135.140	−87.577	0.00	−468.04	−87.283	0.34
1493	1e+1	3	13	13.69	−41.804	3.14	−47.239	−43.160	0.00	−395.69	−43.160	0.00
1507	1e+0	6	13	10.31	−8.295	0.08	−49.709	−8.301	0.00	−44.37	−8.301	0.00
1535	2e+0	3	23	83.47	−11.241	2.98	−13.407	−11.586	0.00	−107.86	−11.398	1.62
1619	2e+0	3	20	35.62	−9.213	0.05	−10.302	−9.217	0.00	−74.55	−9.217	0.00
1661	1e+0	3	8	35.85	−15.666	1.81	−19.667	−15.955	0.00	−139.25	−15.955	0.00
1675	1e+1	3	11	41.30	−75.537	0.17	−96.864	−75.669	0.00	−435.48	−75.669	0.00
1703	2e+1	5	22	62.63	−131.330	1.11	−180.935	−132.802	0.00	−929.92	−132.802	0.00
1745	5e+0	4	19	40.44	−72.351	0.04	−77.465	−72.377	0.00	−317.99	−72.377	0.00
1773	5e+0	1	56	120.65	−14.176	3.19	−21.581	−14.642	0.00	−118.65	−14.642	0.00
1886	2e+1	1	35	28.19	−78.620	0.07	−135.615	−78.672	0.00	−324.87	−78.672	0.00
1913	5e+0	4	18	15.10	−51.879	0.44	−68.555	−52.109	0.00	−164.26	−51.348	1.46
1922	1e+1	1	26	13.22	−35.451	1.39	−121.872	−35.951	0.00	−123.2	−35.951	0.00
1931	1e+1	1	13	8.59	−53.709	3.59	−85.196	−55.709	0.00	−204.08	−54.290	2.55
1967	5e+1	1	38	33.01	−105.616	1.83	−136.098	0.000	100	−622.57	−107.581	0.00
Max	100	6	56	120.65		13.17			100			3.49

Table 5 Sequential penalized SDP

Inst	Sequential SDP						BARON			COUENNE		
	η	i^{feas}	i^{stop}	t (s)	UB	GAP (%)	LB	UB	GAP (%)	LB	UB	GAP (%)
0343*	1e+2	1	53	29.24	−6.379	0.12	−95.372	−6.386	0.00	−7668.005	−6.386	0.00
0911	2e+0	1	9	5.19	−31.811	1.05	−172.777	0.000	100	−172.777	−31.026	3.49
0975	2e+0	2	13	8.18	−37.845	0.02	−47.428	−37.794	0.16	−171.113	−36.812	2.75
1055	5e+0	1	8	4.36	−32.528	1.54	−37.841	−33.037	0.00	−199.457	−33.037	0.00
1143	5e+0	4	15	7.89	−55.606	2.87	−69.522	−57.247	0.00	−384.45	−53.367	6.78
1157	1e+0	1	5	3.15	−10.945	0.03	−11.414	−10.948	0.00	−80.51	−10.948	0.00
1353*	1e+0	1	10	6.12	−7.712	0.03	−7.925	−7.714	0.00	−73.28	−7.714	0.00
1423*	1e+0	1	5	3.28	−14.676	1.95	−16.313	−14.968	0.00	−76.13	−14.078	5.94
1437*	1e+0	1	7	4.30	−7.787	0.03	−9.601	−7.789	0.00	−87.58	−7.789	0.00
1451†	5e+0	2	6	5.09	−85.972	1.83	−135.140	–	-	−468.04	–	–
1493*	5e+0	1	6	4.10	−43.160	0.00	−47.239	−43.160	0.00	−395.69	−43.160	0.00
1507	5e−1	3	6	3.28	−8.291	0.12	−49.709	−8.301	0.00	−44.37	−8.301	0.00
1535	1e+0	1	16	13.05	−11.363	1.93	−13.407	−11.397	1.63	−107.86	−11.398	1.63
1619*	1e+0	1	7	4.64	−9.213	0.05	−10.302	−9.217	0.00	−74.55	−9.217	0.00
1661*	1e+0	1	12	7.57	−15.955	0.00	−19.667	−15.955	0.00	−139.25	−15.955	0.00
1675*	5e+0	1	5	3.75	−75.550	0.16	−96.864	−75.669	0.00	−435.48	−75.669	0.00
1703†	1e+1	1	10	6.96	−132.539	0.20	−180.935	−131.466	1.01	−929.92	–	–
1745	5e+0	1	8	4.75	−71.828	0.76	−77.465	−72.377	0.00	−317.99	−72.377	0.00
1773*	1e+0	1	8	5.44	−14.633	0.06	−21.581	−14.642	0.00	−118.65	−14.636	0.04
1886	5e+0	2	9	5.84	−78.659	0.02	−135.615	−49.684	36.84	−324.87	−78.672	0.00
1913	5e+0	1	20	12.48	−51.866	0.47	−68.555	−52.109	0.00	−164.26	−51.348	1.46
1922*	5e+0	1	7	4.34	−35.452	1.39	−121.872	−35.916	0.10	−123.2	−35.951	0.00
1931	5e+0	1	10	5.87	−54.894	1.46	−85.196	−55.709	0.00	−204.08	−54.290	2.55
1967	1e+1	1	6	5.49	−104.752	2.63	−136.098	0.000	100	−622.57	−107.581	0.00
Max	100	4	53	29.24		2.87			100			6.78

† Rows 1451 and 1703 are excluded from maximum computations due to missing entries. * $i^{\text{feas}} = 1$ is predicted by Theorem 2

Table 6 Sequential penalized SDP + RLT

Inst	Sequential SDP + RLT						BARON			COUENNE		
	η	i^{feas}	i^{stop}	t (s)	UB	GAP (%)	LB	UB	GAP (%)	LB	UB	GAP (%)
0343	0e+0	0	0	1.42	−6.386	0.00	−95.372	−6.386	0.00	−7668.005	−6.386	0.00
0911	2e−1	4	5	13.08	−32.147	0.00	−172.777	0.000	100	−172.777	−31.026	3.49
0975	2e−1	3	5	12.75	−37.852	0.00	−47.428	−37.794	0.16	−171.113	−36.812	2.75
1055	1e+0	5	8	9.56	−32.874	0.49	−37.841	−33.037	0.00	−199.457	−33.037	0.00
1143	5e−1	4	5	7.27	−57.241	0.01	−69.522	−57.247	0.00	−384.45	−53.367	6.78
1157	0e+0	0	0	0.88	−10.948	0.00	−11.414	−10.948	0.00	−80.51	−10.948	0.00
1353	0e+0	0	0	0.45	−7.714	0.00	−7.925	−7.714	0.00	−73.28	−7.714	0.00
1423	2e−1	1	2	2.82	−14.929	0.25	−16.313	−14.968	0.00	−76.13	−14.078	5.94
1437	1e−2	1	2	7.02	−7.789	0.00	−9.601	−7.789	0.00	−87.58	−7.789	0.00
1451	2e+0	2	5	24.45	−87.573	0.01	−135.140	−87.577	0.00	−468.04	−86.860	0.82
1493	5e−1	1	2	2.76	−43.160	0.00	−47.239	−43.160	0.00	−395.69	−43.160	0.00
1507	0e+0	0	0	0.61	−8.301	0.00	−49.709	−8.301	0.00	−44.37	−8.301	0.00
1535	5e−1	1	10	38.01	−11.536	0.43	−13.407	−11.397	1.63	−107.86	−11.398	1.62
1619	0e+0	0	0	2.38	−9.217	0.00	−10.302	−9.217	0.00	−74.55	−9.217	0.00
1661	1e−1	1	2	12.88	−15.955	0.00	−19.667	−15.955	0.00	−139.25	−15.955	0.00
1675	5e−1	4	0	4.22	−75.669	0.00	−96.864	−75.669	0.00	−435.48	−75.669	0.00
1703[†]	2e+0	1	3	13.50	−72.376	0.00	−77.465	−	–	−317.99	−72.377	0.00
1773	2e−1	3	4	18.01	−14.626	0.11	−21.581	−14.642	0.00	−118.65	−14.636	0.04
1886	2e+0	2	4	9.05	−78.643	0.04	−135.615	−78.672	0.00	−324.87	−78.672	0.00
1913	1e+0	2	6	11.49	−52.108	0.00	−68.555	−52.109	0.00	−164.26	−51.348	1.46
1922	2e+0	1	5	3.35	−35.556	1.10	−121.872	−35.741	0.58	−123.2	−35.951	0.00
1931	1e+0	1	2	2.99	−55.674	0.06	−85.196	−53.760	3.50	−204.08	−54.290	2.55
1967	5e+0	1	8	16.11	−107.052	0.49	−136.098	0.000	100	−622.57	−107.581	0.00
Max	5	5	10	38		1.1		0.000	100			6.78

[†] Row 1703 is excluded from maximum computations due to missing entries

Fig. 2 Convergence of sequential 2×2 SDP, 2×2 SDP + RLT, SDP, and SDP + ,RLT for inst. 1507
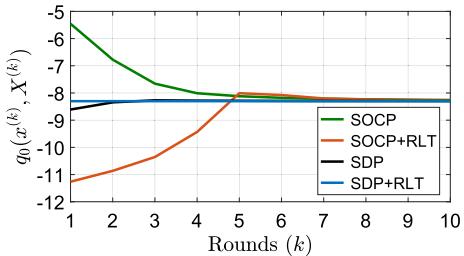

Figure 2, shows the convergence of Algorithm 1 for cases 1507. The choice of η for all curves are taken from the corresponding rows of the Tables 3, 4, 5, and 6.

4.1.2 Choice of the penalty parameter η

In this experiment the sensitivity of different penalization methods to the choice of the penalty parameter η is tested. To this end, one round of the penalized SDP (5a)–(5d) is solved for a wide range of η values. The benchmark case 1143 is used for this experiment. If η is small, none of the proposed penalized SDPs are tight for the case 1143. As the value of η increases, the feasibility violation $\text{tr}\{\overset{*}{X} - \overset{*}{x}\overset{*}{x}^{\top}\}$ abruptly vanishes once crossing $\eta = 1.9$, $\eta = 7.7$, and $\eta = 19.6$, for the penalized 2×2 SDP, SDP and SDP + RLT, respectively. Remarkably, if $\overset{*}{x}^{\text{SDP+RLT}}$ is used as the initial point and $\eta \simeq 2$, then the penalized SDP + RLT (5a)–(5d) produces a feasible point for the benchmark case 1143 whose objective value is within 0.2% of the reported optimal cost $q_0(x^{\text{QPLIB}})$.

Additionally, Fig. 3 shows the result of one round penalized SDP for a wide range of η values, on cases QPLIB 1423, 1675, and 1967. As demonstrated by the figures, the resulting objective values of penalized SDP grow slowly beyond certain limits of η. This indicates that the proposed approach is not very sensitive to the choice of η and a wide range of η values can be used for penalization.

4.2 Large-scale system identification problems

Following [25], this case study is concerned with the problem of identifying the parameters of linear dynamical systems given limited observations and non-uniform snapshots of state vectors. Optimization is an important tool for problems involving dynamical systems such as the identification of transfer functions and control synthesis [26,39,69,78,79]. One of these computationally-hard problems is system identification based solely on data (without intrusive means) which has been widely studied in the literature of control [67,70]. In this case study, we cast system identification as a non-convex QCQP and evaluate the ability of the proposed penalized SDP in solving very large scale instances of this problem.

Consider a discrete-time linear system described by the system of equations:

$$z[\tau + 1] = Az[\tau] + Bu[\tau] + w[\tau] \quad \tau = 1, 2, \ldots, T - 1 \tag{45a}$$

where

- $\{z[\tau] \in \mathbb{R}^n\}_{\tau=1}^{T}$ are the state vectors that are known at times $\tau \in \{\tau_1, \ldots, \tau_o\}$,
- $\{u[\tau] \in \mathbb{R}^m\}_{\tau=1}^{T}$ are the known control command vectors.
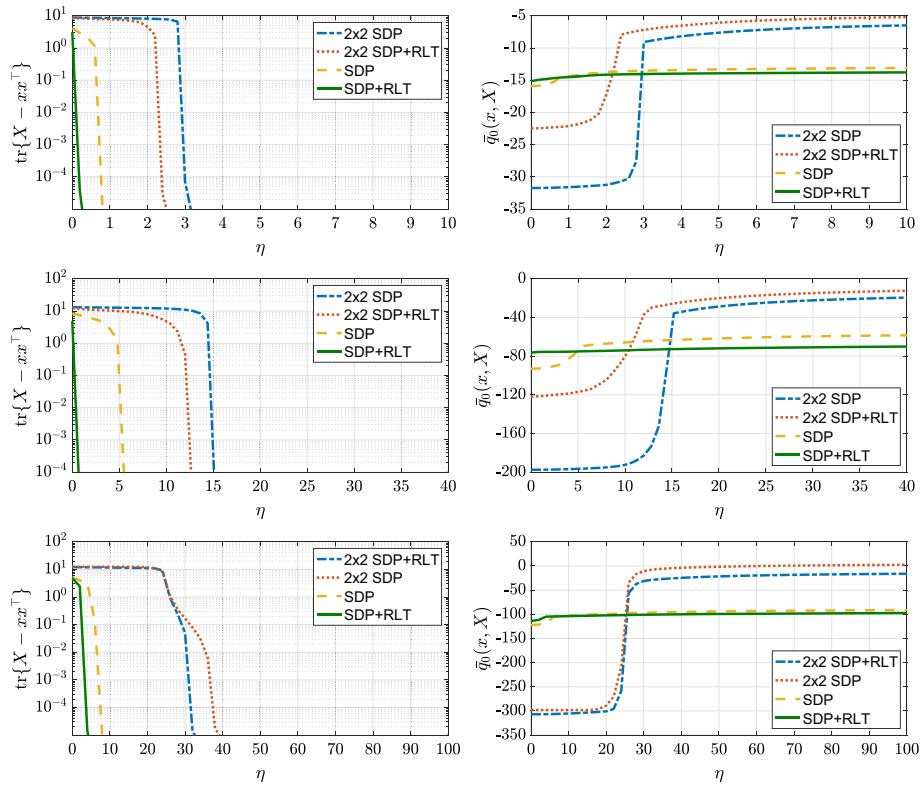
Fig. 3 The effect of η on the performance of penalized 2×2 SDP, 2×2 SDP $+$ RLT, SDP, and SDP $+$ RLT for cases QPLIB 1423, 1675, and 1967

- $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{n \times m}$ are fixed unknown matrices, and
- $\{w[\tau] \in \mathbb{R}^n\}_{\tau=1}^{T}$ account for the unknown disturbance vectors.

Our goal is to estimate the pair of ground truth matrices $(\bar{A}, \bar{B})$, given a sample trajectory of the control commands $\{\bar{u}[\tau] \in \mathbb{R}^n\}_{\tau=1}^{T}$ and the incomplete state vectors $\{\bar{z}[\tau] \in \mathbb{R}^n\}_{\tau \in \{\tau_1, \ldots, \tau_o\}}$. To this end, we employ the minimum least absolute value estimator which amounts to the following QCQP:

$$\underset{\substack{\{y[\tau]\in\mathbb{R}^n\}_{\tau=1}^{T-1} \\ \{z[\tau]\in\mathbb{R}^n\}_{\tau=1}^{T} \\ A\in\mathbb{R}^{n\times n} \\ B\in\mathbb{R}^{n\times m}}}{\text{minimize}} \quad \sum_{\tau=1}^{T-1} \mathbf{1}_n^\top y[\tau] \tag{46a}$$

subject to $\quad y[\tau] \geq +z[\tau+1] - Az[\tau] - B\bar{u}[\tau] \quad \tau \in \{1, 2, \ldots, T-1\}, \tag{46b}$

$\quad y[\tau] \geq -z[\tau+1] + Az[\tau] + B\bar{u}[\tau] \quad \tau \in \{1, 2, \ldots, T-1\}, \tag{46c}$

$\quad z[\tau] = \bar{z}[\tau] \quad \tau \in \{\tau_1, \ldots, \tau_o\}. \tag{46d}$

For every $\tau \in \{1, 2, \ldots, T-1\}$, the auxiliary variable $y[\tau] \in \mathbb{R}^n$ accounts for $|z[\tau+1] - Az[\tau] - B\bar{u}[\tau]|$. This relation is imposed through the pair of constraints (46b) and (46c).

Fig. 4 Convergence of the
sequential penalized 2×2 SDP
for large-scale system
identification with different
disturbance levels
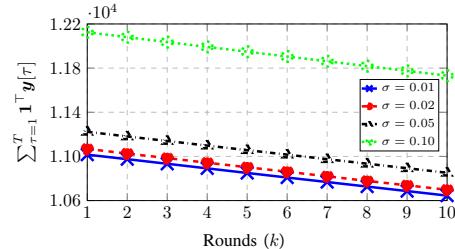
The problem (46a)–(46d), can be cast in the form of (1a)–(1c), with respect to the vector

$$\boldsymbol{x} \triangleq [\boldsymbol{z}[1]^\top, \ldots, \boldsymbol{z}[T]^\top, \text{vec}\{\boldsymbol{A}\}^\top, \alpha \boldsymbol{y}[1]^\top, \ldots, \alpha \boldsymbol{y}[T-1]^\top, \alpha \text{vec}\{\boldsymbol{B}\}^\top], \qquad (47)$$

where α is a preconditioning constant. To solve the resulting problem, we use the sequential Algorithm 1 equipped with the 2×2 SDP relaxation and the initial point $\hat{\boldsymbol{x}} = \boldsymbol{0}$.

We consider system identification problems with $n = 25$, $m = 20$, $T = 500$ and $o = 400$. In every experiment, $\{\tau_1, \ldots, \tau_o\}$ is a uniformly selected subset of $\{1, 2, \ldots, T\}$. The resulting QCQP variable $\boldsymbol{x}$ is 23605-dimensional and the problem is 16100-dimensional if we exclude the known state vectors $\{\bar{\boldsymbol{z}}[\tau] \in \mathbb{R}^n\}_{\tau \in \{\tau_1, \ldots, \tau_o\}}$. Due to sparsity of the QCQP (46a)–(46d) each round of the penalized 2×2 SDP is solved within 30 min, by omitting the elements of the lifted variable $\boldsymbol{X}$ that do not appear in the objective and constraints. All of the convex programs are solved using MOSEK v8.1 [4] through MATLAB 2017a and on a desktop computer with a 12-core 3.0GHz CPU and 256GB RAM. Due to the sheer size of this problem, we were only able to solve instances with $T \leq 70$ using BARON and COUENNE non of which resulted in successful recovery of the unknown matrices due to limited data points.

The ground truth values are chosen as follows:

– The elements of $\bar{\boldsymbol{A}} \in \mathbb{R}^{25 \times 25}$ have zero-mean Gaussian distribution and the matrix is scaled in such a way that the largest singular value is equal to 0.5.
– Every element of $\bar{\boldsymbol{B}} \in \mathbb{R}^{25 \times 20}$, $\{\bar{\boldsymbol{u}}[\tau] \in \mathbb{R}^{20}\}_{\tau=1}^T$ and $\bar{\boldsymbol{z}}[1] \in \mathbb{R}^{25}$ have standard normal distribution.
– The elements of $\{\bar{\boldsymbol{w}}[\tau] \in \mathbb{R}^{25}\}_{\tau=1}^{T-1}$ have independent zero-mean Gaussian distribution with the standard deviation $\sigma \in \{0.01, 0.02, 0.05, 0.10\}$.

For each experiment, we ran Algorithm 1 for 10 rounds. The preconditioning and penalty terms are set to $\alpha = 10^{-3}$ and $\eta = 40$, respectively.

For each $\sigma \in \{0.01, 0.02, 0.05, 0.10\}$, we have run 10 random experiments resulting in the average recovery errors 0.0005, 0.0010, 0.0026, and 0.0062, respectively, for $\frac{1}{n}\|\bar{\boldsymbol{A}} - \boldsymbol{A}^{(10)}\|_F$, and the average errors 0.0014, 0.0028, 0.0070, and 0.0141, respectively, for $(mn)^{-\frac{1}{2}}\|\bar{\boldsymbol{B}} - \boldsymbol{B}^{(10)}\|_F$. In all of the trials, a feasible point is obtained in the first round of Algorithm 1. Figure 4 illustrates the convergence behavior of the objective functions for one of the trials for each disturbance level.

5 Conclusions

This paper introduces a penalization approach for constructing feasible and near-optimal solutions to non-convex quadratically-constrained quadratic programming (QCQP) problems. Given an arbitrary initial point (feasible or infeasible) for the original QCQP, penalized

semidefinite programs are formulated by adding a linear term to the objective. A generalized linear independence constraint qualification (LICQ) condition is introduced as a regularity criterion for initial points, and it is shown that the solution of penalized SDP is feasible for QCQP if the initial point is regular and close to the feasible set. We show that the proposed penalized SDPs can be solved sequentially in order to improve the objective of the feasible solution. Numerical experiments on QPLIB benchmark cases demonstrate that the proposed sequential approach compares favorably with non-convex optimizers BARON and COUENNE. Moreover, the scalability of the proposed method is demonstrated on large-scale system identification problems.

A Application to polynomial optimization

In this section, we show that the proposed penalized SDP approach can be used for polynomial optimization as well. A polynomial optimization problem is formulated as

$$\underset{\boldsymbol{x} \in \mathbb{R}^n}{\text{minimize}} \ u_0(\boldsymbol{x}) \tag{48a}$$

$$\text{s.t.} \quad u_k(\boldsymbol{x}) \leq 0, \qquad k \in \mathcal{I} \tag{48b}$$

$$u_k(\boldsymbol{x}) = 0, \qquad k \in \mathcal{E}, \tag{48c}$$

for every $k \in \{0\} \cup \mathcal{I} \cup \mathcal{E}$, where each function $u_k : \mathbb{R}^n \to \mathbb{R}$ is a polynomial of arbitrary degree. Problem (48a)–(48c) can be reformulated as a QCQP of the form:

$$\underset{\boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{y} \in \mathbb{R}^o}{\text{minimize}} \ w_0(\boldsymbol{x}, \boldsymbol{y}) \tag{49a}$$

$$\text{s.t.} \quad w_k(\boldsymbol{x}, \boldsymbol{y}) \leq 0, \quad k \in \mathcal{I} \tag{49b}$$

$$w_k(\boldsymbol{x}, \boldsymbol{y}) = 0, \quad k \in \mathcal{E} \tag{49c}$$

$$v_i(\boldsymbol{x}, \boldsymbol{y}) = 0, \quad i \in \mathcal{O}, \tag{49d}$$

where $\boldsymbol{y} \in \mathbb{R}^{|\mathcal{O}|}$ is an auxiliary variable, and $v_1, \ldots, v_{|\mathcal{O}|}$ and $w_0, w_1, \ldots, w_{|\{0\} \cup \mathcal{I} \cup \mathcal{E}|}$ are quadratic functions with the following properties:

- For every $\boldsymbol{x} \in \mathbb{R}^n$, the function $\boldsymbol{v}(\boldsymbol{x}, \cdot) : \mathbb{R}^{|\mathcal{O}|} \to \mathbb{R}^{|\mathcal{O}|}$ is invertible,
- If $\boldsymbol{v}(\boldsymbol{x}, \boldsymbol{y}) = \boldsymbol{0}_n$, then $w_k(\boldsymbol{x}, \boldsymbol{y}) = u_k(\boldsymbol{x})$ for every $k \in \{0\} \cup \mathcal{I} \cup \mathcal{E}$.

Based on the above properties, there is a one-to-one correspondence between the feasible sets of (48a)–(48c) and (49a)–(49d). Moreover, a feasible point $(\overset{*}{\boldsymbol{x}}, \overset{*}{\boldsymbol{y}})$ is an optimal solution to the QCQP (49a)–(49d) if and only if $\overset{*}{\boldsymbol{x}}$ is an optimal solution to the polynomial optimization problem (48a)–(48c).

Theorem 3 [51] *Suppose that* $\{u_k\}_{k \in \{0\} \cup \mathcal{I} \cup \mathcal{E}}$ *are polynomials of degree at most d, consisting of m monomials in total. There exists a QCQP reformulation of the polynomial optimization* (48a)–(48c) *in the form of* (49a)–(49d), *where* $|\mathcal{O}| \leq mn \left(\lfloor \log_2(d) \rfloor + 1 \right)$.

The next proposition shows that the LICQ regularity of a point $\hat{\boldsymbol{x}} \in \mathbb{R}^n$ is inherited by the corresponding point $(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}) \in \mathbb{R}^n \times \mathbb{R}^o$ of the QCQP reformulation (49a)–(49d).

Proposition 1 *Consider a pair of vectors* $\hat{\boldsymbol{x}} \in \mathbb{R}^n$ *and* $\hat{\boldsymbol{y}} \in \mathbb{R}^{|\mathcal{O}|}$ *satisfying* $\boldsymbol{v}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}) = \boldsymbol{0}_n$. *The following two statements are equivalent:*

1. $\hat{x}$ *is feasible and satisfies the LICQ condition for the polynomial optimization problem* (48a)–(48b).
2. $(\hat{x}, \hat{y})$ *is feasible and satisfies the LICQ condition for the QCQP* (49a)–(49d).

Proof From $u(\hat{x}) = w(\hat{x}, \hat{y})$ and the invertiblity assumption for $v(\hat{x}, \cdot)$, we have

$$\frac{\partial u(\hat{x})}{\partial x} = \left[\frac{\partial w(\hat{x}, \hat{y})}{\partial x} \; \frac{\partial w(\hat{x}, \hat{y})}{\partial y} \right] \left[I - \left(\frac{\partial v(\hat{x}, \hat{y})}{\partial y} \right)^{-1} \frac{\partial v(\hat{x}, \hat{y})}{\partial x} \right]^\top$$
$$= \frac{\partial w(\hat{x}, \hat{y})}{\partial x} - \frac{\partial w(\hat{x}, \hat{y})}{\partial y} \left(\frac{\partial v(\hat{x}, \hat{y})}{\partial y} \right)^{-1} \frac{\partial v(\hat{x}, \hat{y})}{\partial x}. \tag{50}$$

Therefore, $\mathcal{J}_{\text{PO}}(\hat{x}) = \frac{\partial u(\hat{x})}{\partial x}$ is equal to the Schur complement of

$$\mathcal{J}_{\text{QCQP}}(\hat{x}, \hat{y}) = \begin{bmatrix} \frac{\partial w(\hat{x}, \hat{y})}{\partial x} & \frac{\partial w(\hat{x}, \hat{y})}{\partial y} \\ \frac{\partial v(\hat{x}, \hat{y})}{\partial x} & \frac{\partial v(\hat{x}, \hat{y})}{\partial y} \end{bmatrix}, \tag{51}$$

which is the Jacobian matrix of the QCQP (49a)–(49d) at the point $(\hat{x}, \hat{y})$. As a result, the matrix $\mathcal{J}_{\text{PO}}(\hat{x})$ is singular if and only if $\mathcal{J}_{\text{QCQP}}(\hat{x}, \hat{y})$ is singular. $\square$

B Reformulation-linearization technique

This appendix covers the reformulation-linearization technique (RLT) of Sherali and Adams [72] as an approach to strengthen convex relaxations of the form (4a)–(4d) in the presence of affine constraints. Define $\mathcal{L}$ as the set of affine constrains in the QCQP (1a)–(1c), i.e., $\mathcal{L} \triangleq \{k \in \mathcal{I} \cup \mathcal{E} \mid A_k = \mathbf{0}_{n \times n}\}$. Define also

$$H \triangleq [B\{\mathcal{L} \cap \mathcal{I}\}^\top, B\{\mathcal{L} \cap \mathcal{E}\}^\top, -B\{\mathcal{L} \cap \mathcal{E}\}^\top]^\top, \tag{52a}$$
$$h \triangleq [c\{\mathcal{L} \cap \mathcal{I}\}^\top, c\{\mathcal{L} \cap \mathcal{E}\}^\top, -c\{\mathcal{L} \cap \mathcal{E}\}^\top]^\top, \tag{52b}$$

where $B \triangleq [b_1, \ldots, b_{|\mathcal{I} \cap \mathcal{E}|}]^\top$ and $c \triangleq [c_1, \ldots, c_{|\mathcal{I} \cap \mathcal{E}|}]^\top$. Every $x \in \mathcal{F}$ satisfies

$$Hx + h \leq 0, \tag{53}$$

and, as a result, all elements of the matrix

$$Hxx^\top H^\top + hx^\top H^\top + Hxh^\top + hh^\top \tag{54}$$

are non-negative if x is feasible. Hence, the inequality

$$e_i^\top V(x, xx^\top) e_j \geq 0 \tag{55}$$

holds true for every $x \in \mathcal{F}$ and $(i, j) \in \mathcal{H} \times \mathcal{H}$, where $V : \mathbb{R}^n \times \mathbb{S}_n \to \mathbb{S}_{|\mathcal{H}|}$ is defined as

$$V(x, X) \triangleq HXH^\top + hx^\top H^\top + Hxh^\top + hh^\top, \tag{56}$$

$\mathcal{H} \triangleq \{1, \ldots, |\mathcal{L} \cap \mathcal{I}| + 2|\mathcal{L} \cap \mathcal{E}|\}$, and $e_1, \ldots, e_{|\mathcal{H}|}$ denote the standard bases in $\mathbb{R}^{|\mathcal{H}|}$.

This leads to a strengthened relaxation of QCQP (1a)–(1c):

$$\underset{x \in \mathbb{R}^n, X \in \mathbb{S}_n}{\text{minimize}} \quad \bar{q}_0(x, X) \tag{57a}$$

$$\text{s.t.} \quad \bar{q}_k(x, X) \leq 0, \qquad k \in \mathcal{I} \tag{57b}$$

$$\bar{q}_k(x, X) = 0, \qquad k \in \mathcal{E} \tag{57c}$$

$$X - xx^\top \succeq_{\mathcal{C}_r} 0 \tag{57d}$$

$$e_i^\top V(x, X)e_j \geq 0, \qquad (i, j) \in \mathcal{V} \tag{57e}$$

where $\mathcal{V} \subseteq \mathcal{H} \times \mathcal{H}$ is a selection of RLT inequalities.

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